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FAST SCANNING AND FAST IMAGE RECONSTRUCTION IN ATOMIC FORCE MICROSCOPY

AF FA9550-06-1-0252

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Abstract

This project aims at addressing challenges of high throughput applications of microcantilever based devices which are predicted to have enormous impact on science, technology, and applications that include various defense applications. This project addresses the challenges in two steps – (1) to substantially increase the imaging throughput by closely packing an array of microcantilevers for parallel (2) to develop numerical algorithms to construct high resolution images from the scan data (typically corrupted with noise, blurring effects and tip-sample convolutions) that are time and storage memory efficient. With respect to (1), we have developed model microcantilever arrays with strong crosscoupling, compared control design decentralized and distributed controller architectures, presented new theory to analyze stability and performance of spatially and temporally varying plants, studied invariant nominal models and present necessary and sufficient conditions for robustness when the underlying perturbations on them are spatiotemporal varying linear or nonlinear and unstructured or structured. We addressed performance and robustness issues with noisy and failed communications between subcontrollers and issues with performance under switching and reconfiguring. With respect to (2), we developed robust numerical algorithms that solve integral equations defined on irregularly (as opposed to rectangular) shaped domains which model the scan data from most AFM applications.

Background and Motivation: The microcantilever based devices such as atomic force microscopes (AFMs) have had a dramatic impact in fields as diverse as biology, materials science, electrochemistry, tribology, biochemistry, surface physics, and medicine and applications such as genomics, DNA scanning and pathogen evaluation [1-3]. Recent applications relevant to air force research such as combinatorial material investigation (for tailoring material that are light, tough and durable) and combinatorial chemistry (for pathogen detection and combinatorial drug discovery) [4,5] have led to growing research on increasing the bandwidths and throughputs of microcantilever based devices. Most of the research pertaining to this new impetus has been in increasing the bandwidths of single cantilever devices such as AFM to enable new studies in biology, material science and physics. New devices, modes of operations, and control techniques have been proposed to obtain higher bandwidths [6-11].

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In contrast, relatively less work has been done for high throughput devices where large microcantilever arrays are used. The current status of this technology is in the fabrication and implementation stage where various micro electro mechanical systems (MEMS) based cantilever arrays are actuated by capacitative or thermal means (as opposed to optical means in single cantilever devices). It is only a matter of time, evident from the pace of research in this direction propelled by the industry and the academia, when individual actuation and sensing of cantilevers in the array will be commercially available.

Results

Modelling and control design of electrostatically actuated microcantilever arrays [14,22]: A basic model an array of electrostatically actuated microcantilevers that can be put to use for numerous applications was developed. The geometry of the abstract system considered is shown in Figure 1. The system consists of infinitely many microcantilevers connected to a base, each forming a micro-capacitor, with the second rigid plate located underneath the microcantilever. The microcantilever is flexible and can move in the vertical axis, however it is assumed to be rigid along the horizontal axis. The vertical displacement of each microcantilever can be controlled by applying a voltage across the plates. The displacement z of ith microcantilever is described by a second order equation

$$\ddot{z}_{i} + b\dot{z}_{i} + \omega^{2}z_{i} = \frac{\varepsilon_{0}A}{2md^{2}}(1 + \frac{2zi}{d})U_{i}^{2} + \frac{1}{m}\sum_{j\neq i,j=i-1}^{i+1}\gamma_{ij}(z_{i} - z_{i}) + \frac{c_{i}U_{i}}{4\pi m\varepsilon_{0}}\sum_{j\neq i}\frac{c_{j}U_{j}(z_{i} - z_{j})}{r_{ij}^{3}} \quad \text{where the}$$

first forcing term is the electrostatic forces between the plates, the second is the mechanical coupling term (assumed as spring like forces due to interactions with immediate neighbors) and the third is the electrostatic interactions between the cantilever and its neighbors. The input to the

system is the voltage across the capacitor plates and the output is the current $y_i = \frac{d}{dt}(c_i U_i)$,

$$c_i = \frac{\varepsilon_0 A}{d - z_i}$$
, resulting from cantilever deflections in each cantilever. The details can be found in

[10]. These nonlinear equations were linearized about the equilibrium position of the cantilever, zero velocity and a given nominal potential. Then this linearized model was used for control design and the resulting feedback laws were implemented on the nonlinear model. In order to have some benchmark performance index, we first design a H_{∞} centralized controller for an array of eight microcantilevers. However, to increase the practical benefit of an array, a unit which contains a large number of microcantilevers is required. As the design and implementation of a centralized controller for such systems is impractical, we consider the following two control schemes with localized architecture: a) a H_{∞} decentralized controller that completely ignores the dynamics contributed by the neighbors hence treating them as an external disturbance, b) a H_{∞} distributed controller that makes use of information only from its immediate neighbors. The performance of these controllers are tested via simulations on a finite nonlinear model of the system, and compared with the benchmark performance delivered by the centralized controller. The results are elaborated in Figure 1. It is seen that the performance delivered by a distributed controller is quite comparable to the performance delivered by the benchmark scheme of a centralized controller. In comparison, the performance of the decentralized controller degrades by more than 100% in terms of resolution. Based on the achieved resolution and bandwidth of the distributed controller, the device holds high potential for AFM applications in contact mode,

and mechanical tasks such as indenting, cutting, and lithography. We also established robust performance margins for the distributed controller which are verified via simulations on a finite dimensional linear and nonlinear model of the microcantilever system.

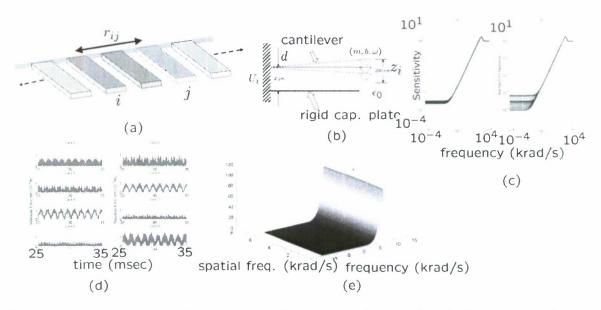


Figure 1: (a) A schematic of the microcantilever array where each unit forms a capacitor as shown in (b). The comparison of sensitivity functions (between the reference signal and tracking error for a cantilever) from taking 10000 neighbors vs 2 neighbors is shown in (c). This explains the efficacy of distributed design using immediate nighbors. The tracking errors on test simulation for 8 cantilevers (with uncertain parameters) shown in (d) with the robust distributed control designs is in the same range as the benchmark centralized system. The robustness analysis uses structural singular values shown in (e) that give conservative bounds on allowed perturbations on the parameters such as natural frequency and damping of the cantilevers.

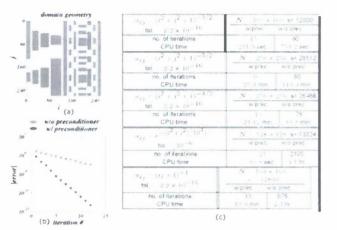
Image reconstruction and deblurring algorithm [12,15]: This problem pertains to developing algorithms for postprocessing of image data arising from AFM scans (or from multicantilever arrays). Since the scanning is done by a tip riding on a sample surface, the resulting image is often blurred due to tip-sample convolution. Also, due to the extremely small scales, other undesirable additive perturbations could lead to images with poor clarity. The main goal in image restoration is to make the processed image to be as close to the true image as possible. The blurring and noise effects are modeled as integral equations of the form $y(\xi) = \int_{\Omega} a(\xi, \xi') x(\xi') d\xi' + n$ where y represents the real image, x represents the original image,

n the noise, and a is called the point spread function which captures the blurring effect. These integral equations result in ill conditioned large matrix equations of the form y = Ax + n where the size of of A is from the order of 10^5 x 10^5 to a few orders higher[12]. The numerical complexity in solving these systems is further compounded by the non rectangular disconnected domains Ω . We have obtained solutions to these large linear systems of equations using preconditioned conjugate gradient method (PCGM) where we have generalized the problem to higher dimensions where Ω is subset of d dimensional euclidean space. In this context, the

cofficient matrix A, is a principal submatrix of a d-level Toeplitz matrix \hat{A} , and the preconditioner for the preconditioned conjugate gradient algorithm is provided in terms of the inverse of a d-level circulant matrix constructed from the elements of A. The preconditioner is shown to yield clustering in the spectrum of the preconditioned matrix which leads to a substantial reduction in the computational cost of solving LRE systems. Analytical results that show that the algorithm can solve the system of equations of size N in $O(N^{(2-1/d)})$ computations.

The results can be found in [12] and some of them are provided in Figure 2.

Figure 2: The algorithm developed allows solving large integral equations over complicated geometries as shown in (a). The preconditioner designed leads convergence (shown in (b)) of the algorithm due to better clustering of the eigenvalues. The table in (c) shows the time efficiency of the proposed algorithms through many examples employed different convolution kernels and domain geometries. The time reductions are as large as 86.8 s from 4.1 hours and 10min from 2.3 hours.



We have made progress in both the aspects of the project, which we lay down in this section. In terms of progress in the control and coordination theme of the problem, we have developed several new theoretical results that deal with various aspects of the analysis and design of spatiotemporal and distributed control systems such as the ones to be used in the AFM arrays. In particular, we have dealt with issues of performance and robustness in the presence of spatiotemporal variations due to imperfections and boundary conditions, issues with noisy and failed communications between subcontrollers as well as issues with performance under switching and reconfiguring.

Noisy and Failed Links [16-19, 23]: We considered two design problems. First, is the case where, without loss of generality, there are two distributed subcontrollers connected to a (generalized) plant and the interest is placed in minimizing the number of noise-free (and dynamics free) communication channels between the subcontrollers needed to provide a given performance. The second is the case where, given a distributed controller designed in the first case, communication noise is present and we seek an optimal choice of the communication signals to guarantee a performance level while keeping the communication signal to noise power limited. We took a linear matrix inequality (LMI) approach to provide solution procedures to these problems and presented examples that demonstrated their efficiency.

We also considered the distributed control of n dynamic agents to optimize an overall system performance metric. Due to limited communication resources, there exist structured interconnections among the agents and the interest is placed on synthesizing a suitably distributed control law to provide a given performance level. Based on a Youla-Kucera (Y-K) parameterization approach, the problem of designing a distributed controller to deliver given

performance levels for different network topologies is shown to be convex in the Y-K parameter Q. Furthermore, if in addition to structured interconnections, packet drops and failures exist in information transmission among the agents, we provided convex conditions to guarantee mean square (MS) stability and to optimize system performance. Also, we have provided convex algorithms to optimize the worst case performance if failures exist.

Switching and Reconfiguring [20, 21]: We considered a distributed system comprised of systems that switch arbitrarily among n stable linear time-invariant (LTI) systems. This can be the case, for example, when a controller is reconfiguring depending on operating conditions. The interest was placed on minimizing the worst case performance of a relevant model matching system over all possible switches with either l_{∞} induced norm or H_2 norm as the performance criterion. This minimization was performed over all Youla-Kucera parameters that switch causally in time among n (stable) LTl systems. For the particular setup at hand, it was shown that the optimal Youla-Kucera parameter need not depend on the switching trajectory in the cases of partially matched switching and unmatched switching, and that it can be obtained as an LTl solution to an associated standard ℓ_1 or H_2 optimization. In the case of matched switching, two convergent sequences to the optimal solution from above and below are formulated in terms of linear programs and quadratic programs respectively for the l_{∞} induced and H_2 norm optimizations. An approximate solution with any given precision is possible by finite truncation. Applications of these results to sensitivity minimization, linear parameter-varying (LPV) control, cooperative control and estimation are provided.

Stability and performance of slowly varying spatiotemporal systems [25-27]: A characterization of stability for slowly varying spatiotemporal systems based on input-output description of the plant and controller was obtained that generalizes the results developed for the standard case for slowly time-varying systems. The controller design considered is based on frozen spatially and temporally invariant descriptions of a spatiotemporal plant. In particular, we considered the case where the controllers are not necessarily adjusted for every instance in space and time, and hence are used for some fixed window in time and space before new controllers are implemented. It was shown that the actual spatiotemporally varying system can be stabilized using frozen in space and time controllers, provided the variations in the spatiotemporal dynamics are sufficiently small. We also showed how the length of these windows enters in the stability analysis. Further it was shown that the l_{∞} performance of such systems cannot be much worse than that of the frozen spatially and temporally invariant systems.

Robustness of Spatially Invariant Systems [24]: We considered spatiotemporal systems and studied their l_{∞} and l_2 robustness properties in the presence of spatiotemporal perturbations. In particular, we considered spatially invariant nominal models and provided necessary and sufficient conditions for system robustness for the cases when the underlying perturbations are linear spatiotemporal varying, and nonlinear spatiotemporal invariant, unstructured or structured. It turned out that these conditions are analogous to the scaled small gain condition (which is equivalent to a spectral radius condition and an LMI for the l_{∞} and l_2 case respectively) derived for standard linear time invariant models subject to time varying linear and time invariant nonlinear perturbations.

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